

194

# JOURNAL OF MOLECULAR SPECTROSCOPY

UNIVERSITY OF HAWAII  
LIBRARY

VOLUME 21, 1966 PERIODICAL

*Edited by*

HARALD H. NIELSEN

*Associate Editor*

K. NARAHARI RAO

*Editorial Advisory Board*

G. Amat

Børge Bak

H. J. Bernstein

Bryce L. Crawford, Jr.

David M. Dennison

H. S. Gutowsky

G. Herzberg

K. K. Innes

Richard C. Lord

P.-O. Löwdin

M. Migeotte

Ian Mills

Robert S. Mulliken

John G. Phillips

John R. Platt

G. B. B. M. Sutherland

H. L. Welsh

E. Bright Wilson, Jr.



**ACADEMIC PRESS**

NEW YORK and LONDON

Copyright© 1966, by Academic Press Inc.

ALL RIGHTS RESERVED

No part of this volume may be reproduced in any form by photostat, microfilm, or any other means, without written permission from the publishers.

*Made in the United States of America*

## CONTENTS OF VOLUME 21

## NUMBER 1, SEPTEMBER 1966

IAN R. BARTKY. The Absorption Spectrum of RbD. Vibrational Numbering of the $A^1\Sigma$ State of RbH.....	1
R. C. WOODS. A General Program for the Calculation of Internal Rotation Splittings in Microwave Spectroscopy.....	4
IAN R. BARTKY. The Absorption Spectrum of Cesium Deuteride. The $A^1\Sigma$ State of CsH.....	25
TEHCHIRO OGAWA AND KOZO HIROTA. Electronic Structure of Diborane and Hyperconjugation Effect.....	29
S. BELL, T. S. VARADARAJAN, A. D. WALSH, P. A. WARSOP, J. LEE, AND L. SUTCLIFFE. Spectrum of Carbon Suboxide in the Ultraviolet.....	42
J. K. WILMSHURST AND J. F. HORWOOD. The Vibrational Spectra and Molecular Structure of Dimethyl Oxalate.....	48
K. K. INNES AND J. E. PARKIN. Band Contour Analyses of the Spectra of Asymmetric Rotor Molecules. Part IV. Analysis of a Type A Band of the Electronic Spectrum of Pyrazine- $h_4$ .....	66
H. D. BIST, J. C. D. BRAND, AND D. R. WILLIAMS. The 2750-Å Electronic Band System of Phenol. Part I. The In-Plane Vibrational Spectrum.....	76

## Notes

J. W. NEBGEN, F. I. METZ, AND W. B. ROSE. A Reinvestigation of the Infrared Spectrum of Gaseous Oxygen Difluoride.....	99
TAISUKE YOSHIOKA AND ALAN G. MACDIARMID. Nuclear Magnetic Resonance Coupling Constant Relationships in Analogous Ethyl, Disilanyl, Silylmethyl, and Methylsilyl Compounds.....	103
J. PLÍVA, V. ŠPIRKO, AND S. TOMAN. Analysis of NMR Spectra by Damped Least Squares.....	106
M. VALEK AND R. LINN BELFORD. A Survey of Temperature Effects, Polarization, and Structure in Crystal Spectra of Some Transition Metal Chelates and Salts.....	108
M. D. OLMAN AND C. D. HAUSE. Molecular Constants of Nitric Oxide from the Near Infrared Spectrum.....	111
Papers Accepted for Publication.....	112

## NUMBER 2, OCTOBER 1966

S. BESNAÏNOU, BRYAN THOMAS, AND S. BRATOŽ. A Theoretical Study of the Characteristic CN Infrared Band.....	113
--	-----



H. L. SCHLAFFER, H. GAUSMANN, AND H. WITZKE. Phosphorescence $^2E_g \rightarrow ^4A_{2g}$ of Molybdenum (III) Complexes.....	125
CHUNG-WANG LUI AND BYRON T. DARLING. Barrier Penetration in the $^{16}O_3$ Molecule. Part II.....	130
BYRON T. DARLING AND CHUNG-WANG LUI. The Upper Electronic State of the $^{16}O_3$ Molecule.....	146
H. P. BENZ, A. BAUDER, AND HS. H. GÜNTARD. Exact Quadrupole Interaction Energies in Rotational Spectra.....	156
H. P. BENZ, A. BAUDER, AND HS. H. GÜNTARD. Microwave Spectrum, Quadrupole Coupling Constants, and Barrier to Internal Rotation of 2-Bromopropene.....	165
BARBRA LAFON AND J. RUD NIELSEN. Normal Coordinate Analysis of $CF_3-CH_3$ and $CF_3-CD_3$ .....	175
S. M. LEE AND W. H. SHAFFER. A New Treatment of the Normal Vibrations of A Linear Diatomic Lattice.....	183
J. V. FOLTZ, D. H. RANK, AND T. A. WIGGINS. Determinations of Some Hydrogen Molecular Constants.....	203
HIROAKI TAKAHASHI, KARL MAMOLA, AND EARLE K. PLYLER. Effects of Hydrogen Bond Formation on Vibrations of Pyridine, Pyrazine, Pyrimidine and Pyridazine.....	217
Notes	
F. JENČ. Possible Solution of Some Problems in Molecular Spectroscopy	231
RICHARD H. COX AND STANFORD L. SMITH. Solvent Dependent H—H Couplings in 2,2-Dichlorocyclopropylbenzene.....	232
Letter to the Editors	
J. M. READ, JR., R. E. MAYO, AND J. H. GOLDSTEIN. Analysis of $^{13}C-H$ Satellite Spectrum of Benzene.....	235
Announcement.....	237
Erratum.....	238
Papers Accepted for Publication.....	239

### NUMBER 3, NOVEMBER 1966

V. F. BYSTROV AND A. U. STEPANYANTS. The Stereochemical Significance of the Long-Range Proton Spin Coupling Constant of the $\sigma$ -Fragment $H-C-C-C-H$ .....	241
F. E. WELSH, F. I. METZ, AND W. B. ROSE. Electron Paramagnetic Resonance Spectra of the $\cdot O_2F$ Radical in Liquid and Solid $O_2F_2$ .....	249
V. S. WATTS AND J. H. GOLDSTEIN. The Effect of Aromatic Solvents on the NMR Parameters of $\alpha$ -Chloroacrylonitrile.....	260
TAIJI KITAGAWA, HIROO INOKUCHI, AND KUMASABURO KODERA. Photoionization of Polycyclic Aromatic Compounds in Vacuum Ultraviolet Region. Azulene.....	267
KÖZÖ INUZUKA AND TOSHIO YOKOTA. Electronic Spectra and Structures of 2,3-Benzotropone, 4,5-Benzotropone, and 4,5-Naphthotropone....	272

ROBIN S. McDOWELL. The $\nu_3$ Infrared Bands of $C^{12}H_4$ and $C^{13}H_4$ .....	280
P. ALSTON STEINER AND W. GORDY. Precision Measurement of Dipole Moments and Other Spectral Constants of Normal and Deuterated Methyl Fluoride and Methyl Cyanide.....	291
V. S. GRIFFITHS AND G. SOCRATES. An NMR Study of Hydrogen-Bonding in Substituted Phenols.....	302
J. G. ANGUS AND G. C. MORRIS. Ionization Potential of the Anthracene Molecule from Rydberg Absorption Bands.....	310
Notes	
DAVID NAEGLI AND HOWARD S. PALMER. Chemiluminescent Emission Spectra of Tin Mono- and Di-Halides.....	325
M. HALMANN, I. LAULICHT, AND J. I. STEINFELD. Franck-Condon Calculations for Iodine Using a Morse Potential.....	328
ROGER E. RONDEAU AND LARRY A. HARRAH. Conformational Analyses in Allyl Halides.....	332
Letter to the Editors	
M. KINOSHITA, B. N. SRINIVASAN, AND S. P. MCGLYNN. Rise-Times of Phosphorescence and Delayed Fluorescence.....	335
Papers Accepted for Publication.....	337

#### NUMBER 4, DECEMBER 1966

G. W. KING AND A. W. RICHARDSON. The Ultraviolet Absorption of Cyanogen Halides. Part I. Identification and Correlation.....	339
G. W. KING AND A. W. RICHARDSON. The Ultraviolet Absorption of Cyanogen Halides. Part II. Analysis of the <i>B</i> and <i>C</i> Systems.....	353
S. TOMAN AND J. PLÍVA. Multiplicity of Solutions of the Inverse Secular Problem.....	362
STURE FORSÉN, BO GESTBLOM, RAGNAR A. HOFFMAN, AND SÖREN RODMAR. An NMR Study of 1-Indanone. Analysis of $A_2B_2$ Spectra.....	372
C. DI LAURO AND I. M. MILLS. Coriolis Interactions about <i>X-Y</i> Axes in Symmetric Tops.....	386
JAMES F. BEECHER. Microwave Spectrum, Dipole Moment, Structure, and Internal Rotation of Dimethyl Selenide.....	414
Papers Accepted for Publication.....	425
Author Index.....	426
Subject Index.....	428

